# Lehrstuhl für Theoretische Chemie

# Ruhr-Universität Bochum

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## Theoretical Chemistry Colloquia (WS 2005/2006)

Time: wednesdays 14:15, Location: Seminarraum NC 03/399

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| 19. 10. 2005 | **Falk Renth**, Physikalische Chemie, Universität Kiel<br>*Photoinduced molecular dynamics of azobenzenes and nucelobases* |
| 26. 10. 2005 | **Ulrich Kleinekathöfer**, Theoretische Physik, Technische Universität Chemnitz<br>*Dynamics in molecular systems: classical and quantum mechanically* |
| 02. 11. 2005 | **Michael Springborg**, Physikalische und Theoretische Chemie, Universität des Saarlandes<br>*Electronic and structural properties of clusters and colloids* |
| 09. 11. 2005 | **Nick Besley**, Department of Chemistry, University of Nottingham<br>*Intracules, electron correlation and excited states* |
| 16. 11. 2005 | **Workshop**, Theoretische Chemie, Ruhr-Universität Bochum<br>*Theoretical approaches to ferredoxins* |
| 23. 11. 2005 | **Michael Resch**, Höchstleistungsrechenzentrum Stuttgart/Universität Stuttgart<br>*Simulation on supercomputers - a key technology for Europe?* |
| 30. 11. 2005 | **Matthias Ullmann**, Biopolymere, Universität Bayreuth<br>*Electrostatic regulation of protein action*<br>(Joint seminar with FOR 436 "Water at Interfaces") |
| 07. 12. 2005 | **Konstantinos Kotsis**, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum<br>*Ab initio calculations of O1S XPS spectra of bulk ZnO and ZnO surfaces* |
| 14. 12. 2005 | **Hardy (E.K.U.) Gross**, Theoretische Physik, Freie Universität Berlin<br>*Density functional theory beyond the Born-Oppenheimer approximation* |
| 21. 12. 2005 | **Tillmann Klamroth**, Theoretische Chemie, Universität Potsdam<br>*Correlated many-electron dynamics in molecules and metallic model systems* |
| 11. 01. 2006 | **Peter Vöhringer**, Physikalische und Theoretische Chemie, Universität Bonn<br>*Femtosecond spectroscopy of electronic and vibrational excitations in hydrogen-bonded fluids*<br>(Joint seminar with FOR 436 "Water at Interfaces") |
| 18. 01. 2006 | **Michael Filatov**, Theoretische Chemie, Universität Groningen<br>*Non-dynamic electron correlation in DFT: perspectives of the ensemble approach* |
| **Special date**<br>**Tu 24.** 01. 2006<br>11:15, NC 5/99 | **Angelos Michaelides**, Abteilung Theorie, Fritz-Haber-Institut, Berlin<br>*Simulating ice nucleation from first principles*<br>(Joint seminar with SFB 558 "Heterogeneous Catalysis") |
| 01. 02. 2006 | **Frank Lechermann**, Centre de Physique Théorique, École Polytechnique, Palaiseau<br>*An introduction to the dynamical mean field approach to the electronic structure of correlated materials*<br>(Joint seminar with SFB 558 "Heterogeneous Catalysis") |
| **Special date**<br>**Tu 07.** 02. 2006<br>11:15, NC 5/99 | **Carmen Sousa**, Departament de Química Física, Universitat de Barcelona<br>*Ab initio studies of defects in bulk and surface oxides. Metal clusters supported on the MgO surface*<br>(Joint seminar with SFB 558 "Heterogeneous Catalysis") |
| **Special date**<br>**Mo 20.** 02. 2006<br>**Time: 14.15** | **Sergei Ivanov**, V. A. Fock Physics Research Institute, Saint-Petersburg State University<br>*Developing Bead-Fourier Path Integral Molecular Dynamics* |
| **Special date**<br>**Th 23.** 02. 2006<br>**Time: 14.00** | **Pawel Rodziewicz**, Chemistry, University of Leiden<br>*Blue-shifted hydrogen bonds* |
| **Special date**<br>15. 03. 2006<br>**Time: 14.15** | **Diedrich T. F. Möhlmann**, DLR-Institut für Plantetenforschung<br>*Water on Mars: presence, consequences, and challenges*<br>(Joint seminar with FOR 436 "Water at Interfaces") |
| **Special date**<br>**Th 16.** 03. 2006<br>**Time: 14.15** | **Christof Drechsel-Grau**, Département de Chimie at École Normale Supérieure, Paris<br>*Environmental effects on conical intersections: a model study of ethylen* |

gez. Die Dozenten der Theoretischen Chemie

**Visitors are welcome to the seminar.**